NOTE

A DATA-ACQUISITION ALGORITHM FOR AUTOANALYSIS SYSTEMS[1]

J. E. PARSONS, T. A. MATHEY, AND A. M. KIRBY

*Coastal Plains Soil and Water Conservation Research Center, P. O. Box 3039, Florence,
South Carolina 29502*

ABSTRACT

Algorithms are presented for computer acquisition of data from an autoanalysis system. These algorithms are implemented using an HP9825 computer-data-acquisition system and a Technicon Auto-Analyzer. In addition to providing accurate digital records, the algorithm has saved approximately 25 percent of the time required to record and enter the data into a computer for further statistical and data analyses.

INTRODUCTION

Automatic analytical systems are used to perform many types of chemical analyses. A continuous-flow, automated-analysis system (AA), Technicon Auto-Analyzer II,[2] is used in the laboratory to perform many different chemical analyses. A colorimeter-type detector determines the concentration of several different light-absorbing compounds and provides a signal output to a strip chart recorder and a telemetry output for monitoring the system remotely. Since all analytical steps and conditions are precisely controlled, uniformity is maintained for a large number of samples.

With both automated analytical systems and manual analytical techniques, considerable time is expended converting the data to a digital form and entering these data into a computer for statistical analyses (Bibbero 1977). Interfacing the AA system to a desktop computer can reduce the time required for these functions.

The desktop-computer-based data-acquisition system (DAS) is a Hewlett-Packard 9825A desktop computer with a Hewlett Packard instrument bus (HP-IB), 3455A 40-channel scanner, a 3495A digital voltmeter (DVM), and a 59308A timing generator (TIMER) (Fig. 1). The desktop computer is programmed in Hewlett-Packard's

[2] Mention of tradenames is for reference and does not constitute endorsement by USDA or its cooperators.

HPL language, which is similar to BASIC. Computer software for the DAS was originally written to measure the output data from 20 environment sensors and to provide 30-min summaries of these data.

The AA is interfaced by connecting the telemetry output to a channel on the scanner (Fig. 1). To obtain a reading from the AA system, the DAS system software selects the AA telemetry channel on the scanner and reads the digital voltage output from the DVM.

The AA system is monitored by the computer, so that it runs concurrently with the weather station. The computer software is initiated by an interrupt from the timing generator every 2 sec. At each interrupt, the program decides which tasks have to be performed. One of the tasks is monitoring and measuring the telemetry signal from the AA.

The present AA system can accommodate a maximum of 40 samples/h. To alert the program that a tray of samples is loaded for monitoring and measurement, the AA operator presses a key on the DAS system. Thereafter, at each interrupt, the program executes the AA monitoring subroutine.

MONITORING ALGORITHM

The computer subroutine (a copy of the algorithm is available from the authors) monitors the time derivative of the AA output, $O(t)$, and the time between AA samples. Figure 2 shows a typical chart record of the analogue signal output for six AA samples and a baseline. The time derivative, dO/dt, approximated by the backward difference approximation of the slope of
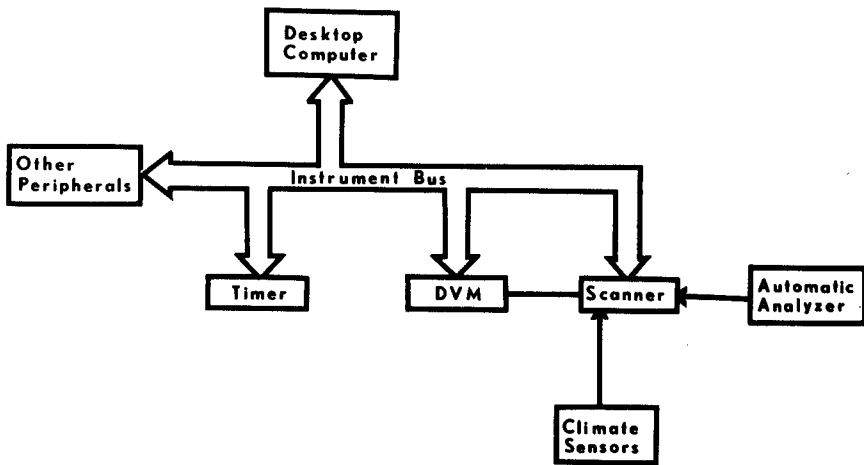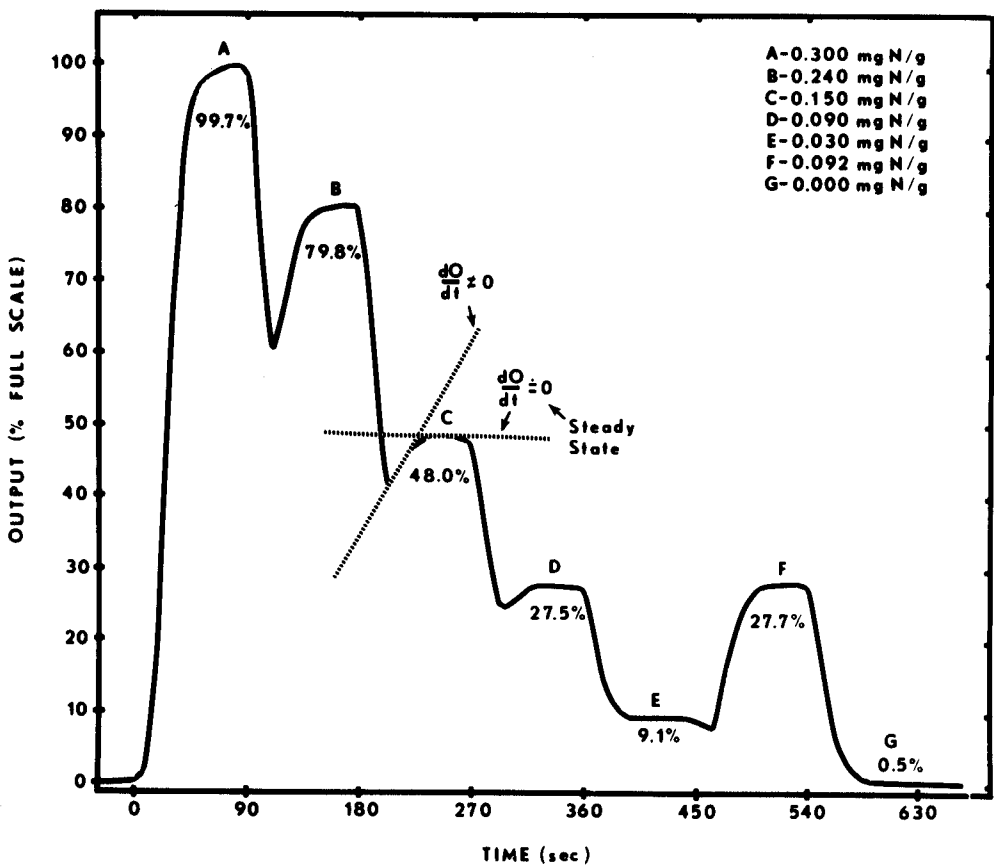
FIG. 1. System configuration.

FIG. 2. Chart recording of the analogue output from six AA samples and a baseline with the DAS digital readings. The letters *A* to *E* are laboratory standards, *F* is a National Bureau of Standards orchard grass, and *G* is the baseline.

the tangent line at that time, O_D. This allows the subroutine to determine when a steady-state plateau has been found. The steady-state level, i.e., the plateau where the time derivative is zero (Fig. 2) is determined by the concentration of the light-absorbing compound in the sample. Since the numerical approximation to the time derivative will be approximately zero during steady state, a constant, ϵ, is used to determine when O_D is approximately zero ($\epsilon = 0.0005$ v/v). The data for the AA sample represent the chemical concentration when $| O_D | <\epsilon$ for 12 sec. At this point, an average steady-state level is computed for the AA sample, based upon the six readings during the 12 sec. After obtaining a steady-state measurement, the routine begins the procedure again for the next AA sample. The steady-state measurements for the six AA samples and the baseline reading, as determined by the DAS, are shown in Fig. 2.

The time between steady-state levels of two AA samples is about 90 sec (Fig. 2). The subroutine uses this time to determine whether a particular AA sample maintained a steady-state level (i.e., $| O_D | <\epsilon$) for the specified 12 sec. If, after 90 sec, the steady-state condition has not been maintained for 12 sec, the subroutine prints a warning of a possible error. The average of the previous six readings is used as the steady-state level for that AA sample, and the readings used in the average are printed along with time derivatives. This enables the operator to check the chart output quickly and diagnose the cause of the faulty reading. Then the subroutine initiates the routine for the next AA sample.

After an AA run has been completed, the DAS data are automatically stored on the internal minicartridge of the DAS system, along with the time of the run. At the end of the day, these data files are transferred to another computer system and permanently stored on disk. Then the data are converted to actual elemental concentrations, reorganized according to the experimental design, and printed in a format usable by the researcher. This permanent storage of the data permits easy recall for further statistical analyses and processing.

SUMMARY

Interfacing to the data-acquisition system proved to be easy and reliable. The essential requirement of this method is a programmable data-acquisition system. The data-acquisition system's requirements are a minimum of one analogue channel with analogue/digital conversion capability in the range of 0 to 5 V DC, the ability to perform measurements at least every 2 sec, and some programming capability to process the data. Small, single-card computer systems that can perform these tasks are available for prices ranging from $2000 to $4000.

This method for automating the output from an automatic analyzer system has many advantages. The operator does not have to record chart output in a form compatible with input into a computer. The data sets do not have to be manually entered into the computer, thus precluding errors in entry. A quick visual scan of the chart output and the digital output from the data-acquisition system can verify the overall system operation. The stored computer data files, the digital computer printouts, and the chart recordings provide permanent records. The data can be processed more quickly, because, shortly after the chemical analysis has been completed, they are stored on another computer and are ready to be summarized.

REFERENCES

Bibbero, R. J. 1977. Microprocessors in instruments and control. Wiley, New York.